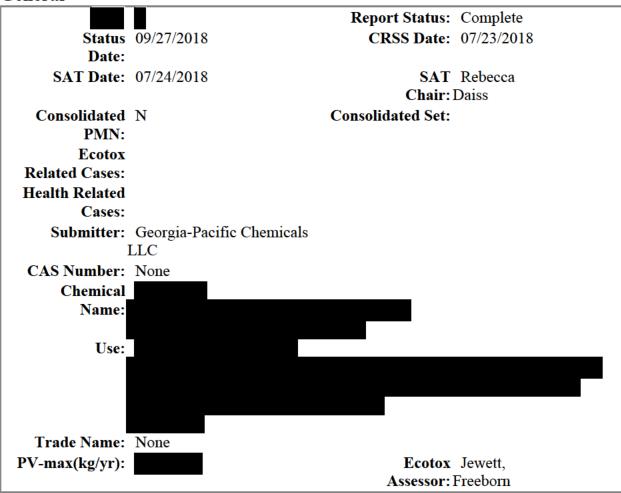
JS 9/13/21 RJA 2/17/22

# **Ecotox Report for Case # P-18-0238**

#### General



# **Fate Summary**

#### **Statement**

Fate P-18-0238 Summary FATE: **Statement:** EPI estimations for the low weight with 1 of each feedstock, MW = Liquid with MP < 25 °C (E) log Kow = -0.98 (E)> 10 g/L at 25 °C (E) $VP < 1.0E-6 \text{ torr at } 25 \text{ }^{\circ}\text{C } (E)$ BP >400 °C (E) H < 1.00E-8 (E) $\log Koc = 1.00 (E)$ log Fish BCF =

0.50 (3) (E)
log Fish BAF = -0.05 (1) (E)
POTW removal (%) = 90-95
via biodeg
Time for complete ultimate aerobic biodeg = wk
Sorption
to soils/sediments = low
PBT Potential: P1B1
\*CEB FATE: Migration to
ground water = negl - slow
Bioconcentration factor to be put into
E-FAST: 1

## **Physical Chemical**

#### **Information**

```
Molecular
        Weight:
    Wt% < 500:
                                   Wt% < 1000:
       Physical Liquid
   State - Neat:
        Melting
                                         Melting
         Point:
                                      Point (est):
            MP NaN °C
         (EPI): (Exp.) 349.8399963378906 °C (Est., Joback) 231.32772827148438 °C (Est.,
                Gold) 255.03018188476562 °C (Est., Selected)
                                          Vapor <0.000001
         Vapor
      Pressure:
                                   Pressure (est):
      VP (EPI): NaN mmHg (Exp.) 8.59551172933426E-19 Pa
                (Est., Antoine) 6.447181807454328E-21 mmHg (Est., Antoine)
                2.9480113791488225E-14 Pa (Est., Grain) 2.2111964860629323E-16
               mmHg
                (Est., Grain) 1.9162998080553697E-10 Pa (Est., Mackay)
                1.4373470305391231E-12 mmHg (Est., Mackay) 2.9480113791488225E-14
                Pa
                (Est., Selected) 2.2111964860629323E-16 mmHg (Est., Selected)
                9.501548522202353E-12 Pa (Est., SubCooled) 7.126767166860948E-14
               mmHg
                (Est., SubCooled)
         Water
                           Water Solubility (est): 1000
     Solubility:
         Water NaN (Exp.) 4009.865234375
Solubility (EPI): (Est.)
 Henry's Law:: NaN atm-m3/mole (Exp.)
                2.1760053648975538E-30 atm-m3/mole (Est., Bond)
```

2.6209289523585576E-38 atm-m3/mole (Est., Group)

**Log** NaN **Log** 2.302585092994046

**Koc (EPI):** (Est., log(MCI)) -2.813410739111778

(Est., log(Kow)) 10.0 L/kg (Est., MCI) 0.05999999865889549 L/kg (Est.,

Kow)

Log NaN (Exp.) -0.22

Kow: Kow (EPI): (Est.)

Log Kow Comment:

#### **SAT Concern Level**

Ecotox 1

**Rating (1):** 

**Ecotox** 

**Rating Comment** 

**(1)**:

**Ecotox Rating** 

(2):

Ecotox

**Rating Comment** 

**(2)**:

Ecotox Route of No releases to

Exposure: water

#### **Ecotox Comments**

**Exposure** Y

**Based Review** 

(Eco):

**Ecotox** 

**Comments:** 

**Exposure Based** 

**Testing:** 

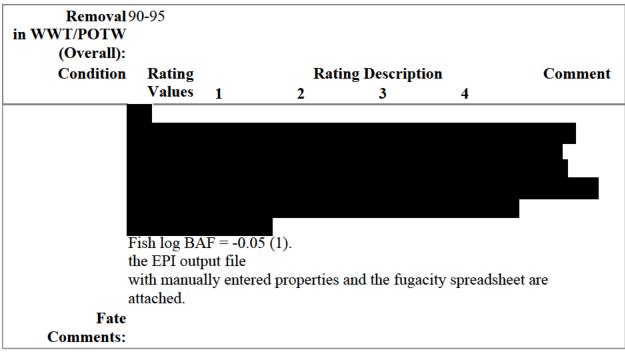
## **PBT Ratings**

Persistence	Bioaccumulation	Toxicity	Comments
1	1		

## **Eco-Toxicity Comment:**

## **Fate Ratings**

Removal	90-95					
in WWT/POTW						
(Overall):	D 4		D 4: 1			<b>C</b>
Condition	Rating Values		_	Description	4	Comment
		1	2	3	4	
Fish BCF:	3.16 L/kg wet-wt					
Log Fish BCF:						
WWT/POTW	1	Low	Moderate	Strong	V. Strong	
Sorption:						
WWT/POTW	4	Extensive	Moderate	Low	Negligible	
Stripping:						
Biodegradation Removal:	2	Unknown	High	Moderate	Negligible	
Biodegradation	2-3	Unknown	Complete	Partial		
<b>Destruction:</b>			*** 1	3.5	3.5	
Aerobic Biodeg Ult:	2	<= Days	Weeks	Months	> Months	
Aerobic Biodeg		<=	Weeks	Months	> Months	
Prim:		Days				
Anaerobic	2	<=	Weeks	Months	> Months	
<b>Biodeg Ult:</b>		Days				
Anaerobic		<=	Weeks	Months	> Months	
<b>Biodeg Prim:</b>		Days				
Hydrolysis (t1/2		<=	Hours	Days	>= Months	
at pH		Minutes				
7,25C) A:			II	D	> = M =41. =	
Hydrolysis (t1/2		<= Minutes	Hours	Days	>= Months	
at pH 7,25C) B:		Millutes				
Sorption to	4	V.	Strong	Moderate	Low	
Soils/Sediments:		Strong	S			
Migration to	1-2	Negligible	Slow	Moderate	Rapid	
<b>Ground Water:</b>						
Photolysis A,		Negligible	Slow	Moderate	Rapid	
Direct:						
Photolysis B,		Negligible	Slow	Moderate	Rapid	
Indirect:		NT 1: '11	C1	N	D '1	
Atmospheric Ox A, OH:		Negligible	Slow	Moderate	Rapid	
Atmospheric Ox		Negligible	Slow	Moderate	Rapid	
B, O3:						
<b>Bio Comments:</b>						



# Ecotoxicity

## Values

Test organism	Test Type	Test Endpoint	Predicted	<b>Experimental Comments</b>
Fish	96-h	LC50	>100	Predictions (for all structures) are based on the Ecological Structure Activity Relationships [ECOSAR] Predictive Model; specifically the QSAR for esters
Daphnid	48-h	LC50	>100	Predictions (for all structures) are based on the Ecological Structure Activity Relationships [ECOSAR]

Test organism	Test Type	Test Endpoint	Predicted	<b>Experimental Comments</b>
				Predictive Model; specifically the QSAR for
Green Algae	96-h	EC50	>100	esters Predictions (for all structures) are based on the Ecological Structure Activity Relationships [ECOSAR] Predictive Model; specifically the QSAR for
Fish	-	Chronic Value	>10	esters Predictions (for all structures) are based on the Ecological Structure Activity Relationships [ECOSAR] Predictive Model; specifically the QSAR for
Daphnid	-	Chronic Value	>10	esters Predictions (for all structures) are based on the Ecological Structure Activity Relationships [ECOSAR] Predictive Model;

Test organism	Test Type	Test Endpoint	Predicted	<b>Experimental Comments</b>
				specifically the QSAR for esters
Green Algae		Chronic Value	>10	Predictions (for all structures) are based on the Ecological Structure Activity Relationships [ECOSAR] Predictive Model; specifically the QSAR for esters
Comments: Ec	cological Stru becifically the 22 (P, dieste a unknown M 53,000 mg/L ( 00% active in	QSAR for esters; Mar/monoether), -2.35 P (P); S = 1E+6 mg (P, diester/monoeth	tionships [E MW ; Lo (P, triester/z /L (P, diester); effective measured c	COSAR] Predictive Model; g Kow = 0.48 (P, diester), monoether); liquid with er and triester/monoether), e concentrations based on oncentrations; hardness <150

# **Ecotox Factors**

Factors	Most Sensitive Endpoint	Assessment Factor	CoC	Comment
Acute Aquatic (ppb):	100000	5	20000	The acute COC is based on the fish/aquatic invertebrate L/EC50 toxicity value (Ecological Structure Activity Relationship [ECOSAR] Predictive Model; specifically the QSAR for esters).
Chronic Aquatic(ppb):	10000	10	1000	The chronic COC is based on the fish/aquatic invertebrate chronic value (Ecological Structure Activity Relationships

Factors	Most Sensitive Endpoint	Assessment Factor	СоС	Comment
				[ECOSAR] Predictive Model; specifically the QSAR for esters).
Factors	Va	lues	Comments	
SARs: I	Esters,			
V	inyl/Allyl/P	ropargyl		
Et	thers	1 01		
SAR Class: I	Esters- inyl/allyl/pro	opargyl		
		terminated		

**Recommended** No testing recommendations

**Testing:** for ecotoxicity **Ecotox** Environmental

Factors Hazard:

**TSCA NCC** 

Category? Esters

Comments: Environmental hazard is relevant to whether a new chemical substance is likely to present unreasonable risk because the significance of the risk is dependent upon both the hazard (or toxicity) of the chemical substance and the extent of exposure to the substance. EPA estimated environmental hazard of this new chemical substance using the Ecological Structure Activity Relationships (ECOSAR) Predictive Model (https://www.epa.gov/tsca-screening-tools/ecological-structure-activity-relationships-ecosar-predictive-model);

specifically the QSAR for esters. Acute toxicity values estimated for fish, aquatic invertebrates and algae are all > 100 mg/L. Chronic toxicity values estimated for fish, aquatic invertebrates, and algae are > 10 mg/L. These toxicity values indicate that the new chemical substance is expected to have low environmental hazard. Application of assessment factors of 5 and 10 to acute and chronic toxicity values, respectively, results in acute and chronic concentrations of concern of 20 mg/L (20,000 ppb) and 1 mg/L (1,000 ppb), respectively.

Environmental Risk:

Risks to the environment were

evaluated by comparing estimated surface water concentrations with the acute and chronic concentrations of concern. Risks to the environmental were not identified based on low hazard.

Potentially Useful

	Information: N/A	
Comments	Telephone Log	
Artifact		Update/Upload
		Time